NANOSCALE ELASTIC PROPERTIES OF DISLOCATIONS AND DISCLINATIONS

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1. Introduction

A correct description of the behavior of defects in thin-film and nanostructured systems needs to take into account both the strong influence of outer and inner interphase boundaries and the fact that the size of a defect core, where classical solutions are singular and incorrect, occurs in the same order as the characteristic length of the system (film thickness, grain size, etc.). To take into account the influence of interphase boundaries, many solutions of boundary value problems for defects have been obtained in the framework of the classical theory of elasticity (see [1–5] for a review). To solve the second problem, some approaches have been proposed which have been aimed at dispensing with classical singularity of elastic fields within defect cores (see [6, 7] for a review). The present paper represents a brief description of our recent results [6–10] dealing with nanoscale elastic fields within and near cores of disclinations [6, 7] and dislocations [6–10] in the framework of gradient elasticity. The main result shown there was an elimination of displacement, strain, stress and energy singularities at the defect line. It is worth noting, that previous continuum models for such kind of defects which have taken into account couple stresses or non-locality (see [6, 7] for a review), do not dispense with the singularity in the displacement or strain field, even though some of them [11–13] claim elimination of stress singularity.

We have started with a simple gradient modification of the linear theory of elasticity in the form [14]

$$\boldsymbol{\sigma} = \lambda(\operatorname{tr}\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon} - c\nabla^2\left[\lambda(\operatorname{tr}\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon}\right], \tag{1}$$

where λ and μ are the Lamé constants, $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the stress and strain tensors, $\boldsymbol{I}$ is the unit tensor, ∇^2 denotes Laplacian and $c > 0$ is the gradient coefficient. Using (1) or similar theory, the authors of [14–20] have demonstrated the elimination of classical singularity from the solution for the strain field at the crack tip.

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Encouraged by these results, we first employed [8, 9] the same gradient theory described by (1) to consider dislocations. In particular, four dislocation configurations (i.e. a screw dislocation, an edge dislocation, and the dipoles of such dislocations) have been considered. It has been shown that in the case of screw dislocation [8], the elastic strain is zero at the dislocation line and achieves a maximum value ($\approx \pm b_z/10\pi\sqrt{c}$), at a distance $\simeq \sqrt{c}$ from it. It is worth noting that for an atomic lattice, the gradient coefficient, c, can be estimated [14] as $\sqrt{c} \approx a/4$, where a is the lattice constant. With the Burgers vector, b_z, taken to be equal to a, it follows that the aforementioned maximum value is estimated as $\approx 12\%$. In the case of edge dislocations [9, 10], we have also shown that all strain components are equal to zero at the dislocation line achieving maximum values (3-14)% within the dislocation core ($r \leq 4\sqrt{c}$).

It has also turned out for both types of dislocations that beyond the dislocation core ($r_0 \simeq 4\sqrt{c}$) the classical and gradient solutions coincide. Furthermore, it has been shown that the total displacement varies smoothly across the dislocation line in contrast to the classical solution which suffers a jump there. In addition, some of the displacement components which are singular in the classical theory now become finite (edge dislocation). We have also considered the displacement and strain distributions for dislocation dipoles and shown that the values of relative displacements of the cut surfaces depend on the dipole arm, in contrast to the classical theory where these displacements are always the same. As a result, two characteristic distances appear naturally in this approach: $r_0 \approx 4\sqrt{c}$ which may be viewed as the radius of dislocation core and $d_0 \approx 10\sqrt{c}$ which may be viewed as the radius of strong short-range nanoscale interaction between dislocations.

In [6], we have considered the elastic fields of disclinations within the gradient theory described by (1). We have found the elastic strains for all kinds of straight disclinations, and examined the interactions between disclinations in dipoles. It has been shown that the main features of the gradient solutions are very similar to the case of dislocations: the singularities at the disclination lines are eliminated from the strain fields which are equal to zero or attain finite values there. The non-vanishing values depend strongly on the dipole arm, d, and exhibit a regular and monotonous (in the case of wedge disclinations) or non-monotonous (in the case of twist disclinations) behavior for short-range nanoscale ($d < 10\sqrt{c}$) interactions between disclinations. When the disclinations annihilate ($d \to 0$), the elastic strains tend to zero value. Far from the disclination line ($r \gg 10\sqrt{c}$) gradient and classical solutions coincide. When $d \ll \sqrt{c}$, the elastic fields of a dipole of wedge disclinations transform into the elastic fields of an edge dislocation [9] as is the case in the classical theory of elasticity.

It is important to emphasize, however, that in the framework of the gradient elasticity theory described by (1), the stress fields of dislocations [8, 9] and disclinations [6] remain as in the classical theory of elasticity (same as in the case of crack problems [14–17, 20]). In order to eliminate the singularities also from the elastic stresses of defects, we used in [7, 10] a more general version of gradient elasticity theory which has been also utilized by Ru and Aifantis [21] (see also

[22]). The constitutive equation of this theory reads

$$\left(1 - c_1\nabla^2\right)\boldsymbol{\sigma} = \left(1 - c_2\nabla^2\right)\left[\lambda(\operatorname{tr}\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon}\right], \tag{2}$$

with two different gradient coefficients c_1 and c_2. In [21] a rather simple mathematical procedure analogous to the one contained in [15] has been outlined for the solution of (2) in terms of solutions of classical elasticity for the same boundary value problem. In fact, it is easily established (see [15], also [6–10]) that the right hand side of (2) for the case of $c_1 \equiv 0$, gives the classical solution for the stress field which we denote here by $\boldsymbol{\sigma}^0$, while the solution for the displacement is determined through the inhomogeneous Helmholtz equation given by

$$\left(1 - c_2\nabla^2\right)\boldsymbol{u} = \boldsymbol{u}^0\,, \tag{3}$$

where $\boldsymbol{u}^0$ denotes the solution of classical elasticity for the same traction boundary value problem. Eq. (3) implies a similar equation for strain, $\boldsymbol{\varepsilon}$, of the gradient theory

$$\left(1 - c_2\nabla^2\right)\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^0\,, \tag{4}$$

in terms of the strain $\boldsymbol{\varepsilon}^0$ of the classical elasticity theory for the same traction boundary value problem. With the displacement or strain field thus determined (which is obviously independent of whether $c_1 \equiv 0$ or $c_1 \neq 0$), it follows that the stress field $\boldsymbol{\sigma}$ of (2) can be determined (for the case $c_1 \neq 0$) from the equation

$$\left(1 - c_1\nabla^2\right)\boldsymbol{\sigma} = \boldsymbol{\sigma}^0\,, \tag{5}$$

where $\boldsymbol{\sigma}^0$ denotes the solution obtained for the same boundary value problem within the classical theory of elasticity.

Thus, in order to solve equation (2), one can solve separately equations (4) and (5) by utilizing the classical solutions $\boldsymbol{\varepsilon}^0$ and $\boldsymbol{\sigma}^0$ provided that appropriate care is taken for the extra (due to the higher order terms) boundary conditions or conditions at infinity. For dislocations and disclinations, this problem's solutions are accounted for by assuming that the strain and stress fields at infinity have the same characteristic features for both the gradient and classical theory. The approach has already been applied [21] to the cases of screw dislocations and mode-III cracks where the asymptotic solutions at the dislocation line and crack tip have been found demonstrating the elimination of both strain and stress singularities there.

Below we report the exact analytical solutions of (2) obtained for straight dislocations and disclinations.

2. Dislocations

2.1. CLASSICAL SOLUTION

Consider a mixed dislocation whose line coincides with the z-axis of a Cartesian coordinate system. Let its Burgers vector be $\boldsymbol{b} = b_x\boldsymbol{e}_x + b_z\boldsymbol{e}_z$ thus determining the edge (b_x) and screw (b_z) components. In the framework of classical elasticity theory, the total displacement field is described by

$$
\begin{aligned}
\boldsymbol{u}^0 &= \frac{b_x \boldsymbol{e}_x + b_z \boldsymbol{e}_z}{2\pi}\left\{\arctan\frac{y}{x} + \frac{\pi}{2}\mathrm{sign}(y)[1-\mathrm{sign}(x)]\right\} \\
&+ \frac{b_x}{4\pi(1-\nu)}\left\{\boldsymbol{e}_x\frac{xy}{r^2} - \boldsymbol{e}_y\left[(1-2\nu)\ln r + \frac{x^2}{r^2}\right]\right\}, \qquad (6)
\end{aligned}
$$

where ν is the Poisson ratio, $r^2 = x^2+y^2$. Here we use a single-valued discontinuous form suggested by de Wit [23]. The elastic strain field ε^0_{ij} reads [23, 24] (in units of $1/[4\pi(1-\nu)]$) by

$$
\begin{aligned}
&\varepsilon^0_{xx} = -b_x y\,[(1-2\nu)r^2 + 2x^2]/r^4, \quad \varepsilon^0_{yy} = -b_x y\,[(1-2\nu)r^2 - 2x^2]/r^4, \\
&\varepsilon^0_{xy} = b_x x(x^2-y^2)/r^4, \quad \varepsilon^0_{xz} = -b_z(1-\nu)y/r^2, \quad \varepsilon^0_{yz} = b_z(1-\nu)x/r^2, \qquad (7)
\end{aligned}
$$

and elastic stress field σ^0_{ij} is [23, 24] (in units of $\mu/[2\pi(1-\nu)]$)

$$
\begin{aligned}
&\sigma^0_{xx} = \varepsilon^0_{xx}(\nu=0), \quad \sigma^0_{yy} = \varepsilon^0_{yy}(\nu=0), \quad \sigma^0_{zz} = \nu(\sigma^0_{xx} + \sigma^0_{yy}), \\
&\sigma^0_{xy} = \varepsilon^0_{xy}, \quad \sigma^0_{xz} = \varepsilon^0_{xz}, \quad \sigma^0_{yz} = \varepsilon^0_{yz}, \qquad (8)
\end{aligned}
$$

Fields (6) (y-component), (7) and (8) are singular at the dislocation line.

The elastic energy W^0 of the dislocation per unit dislocation length is [24]

$$
W^0 = \frac{\mu}{4\pi}\left(b_z^2 + \frac{b_x^2}{1-\nu}\right)\ln\frac{R}{r_0}, \qquad (9)
$$

where R denotes the size of the solid and r_0 is a cut-off radius for the dislocation elastic field near the dislocation line. When $r_0 \to 0$, W^0 becomes singular.

2.2. GRADIENT SOLUTION

Let us now consider the corresponding dislocation fields within the theory of gradient elasticity given by (2). As described in *Section 1*, one can obtain the solution of (2) by solving separately equations (3)–(5). They can be solved [9] by using the Fourier transform method. Omitting intermediate calculations, we give here only the final results. For the total displacements, solution of (3) gives [8, 9]

$$
\begin{aligned}
\boldsymbol{u} &= \boldsymbol{u}^0 - \frac{b_x}{4\pi(1-\nu)}\left\{[\boldsymbol{e}_x\,2xy + \boldsymbol{e}_y\,(y^2-x^2)]\,r^2\Phi_2 + \boldsymbol{e}_y\Phi_0\right\} \\
&+ \frac{b_x\boldsymbol{e}_x + b_z\boldsymbol{e}_z}{2\pi}\,\mathrm{sign}(y)\int_0^{+\infty}\frac{s\sin(sx)}{\frac{1}{c_2}+s^2}e^{-|y|\sqrt{\frac{1}{c_2}+s^2}}\,ds, \qquad (10)
\end{aligned}
$$

where $\boldsymbol{u}^0$ is given by (6), $\Phi_0 = (1-2\nu)\,K_0(r/\sqrt{c_2})$, $\Phi_2 = [2c_2/r^2 - K_2(r/\sqrt{c_2})]/r^4$, $K_n(r/\sqrt{c_2})$ is the modified Bessel function of the second kind and $n = 0, 1, \ldots$ denotes the order of this function.

For the elastic strain, solution of (4) gives [8, 9] $\varepsilon_{ij} = \varepsilon^0_{ij} + \varepsilon^{gr}_{ij}$, where ε^0_{ij} are given by (7) and ε^{gr}_{ij} (in units of $1/[2\pi(1-\nu)]$) by

$$
\begin{aligned}
\varepsilon^{gr}_{xx} &= \ \ b_x y\,[(y^2-\nu r^2)\Phi_1 + (3x^2-y^2)\Phi_2], \quad & \varepsilon^{gr}_{xz} &= \ \ b_z\,(1-\nu) y r^2 \Phi_1/2\,,\\
\varepsilon^{gr}_{yy} &= \ \ b_x y\,[(x^2-\nu r^2)\Phi_1 - (3x^2-y^2)\Phi_2], \quad & \varepsilon^{gr}_{yz} &= -\,b_z\,(1-\nu) x r^2 \Phi_1/2\,,\\
\varepsilon^{gr}_{xy} &= -b_x x\,[y^2\Phi_1 + (x^2-3y^2)\Phi_2], & &
\end{aligned}
\qquad (11)
$$

where $\Phi_1 = K_1(r/\sqrt{c_2})/(\sqrt{c_2}r^3)$. For the stresses, the solution of (5) gives [10] $\sigma_{ij} = \sigma^0_{ij} + \sigma^{gr}_{ij}$, where σ^0_{ij} are given by (8) and σ^{gr}_{ij} (in units of $\mu/[\pi(1-\nu)]$) by

$$
\begin{aligned}
&\sigma^{gr}_{xx} = \varepsilon^{gr}_{xx}(\nu=0, c_2 \leftrightarrow c_1), \quad \sigma^{gr}_{yy} = \varepsilon^{gr}_{yy}(\nu=0, c_2 \leftrightarrow c_1), \quad \sigma^{gr}_{zz} = \nu(\sigma^{gr}_{xx} + \sigma^{gr}_{yy}),\\
&\sigma^{gr}_{xy} = \varepsilon^{gr}_{xy}(c_2 \leftrightarrow c_1), \quad \sigma^{gr}_{xz} = \varepsilon^{gr}_{xz}(c_2 \leftrightarrow c_1), \quad \sigma^{gr}_{yz} = \varepsilon^{gr}_{yz}(c_2 \leftrightarrow c_1).
\end{aligned}
\qquad (12)
$$

The main feature of the solution given by (10)–(12) is the absence of any singularities in the displacement, strain and stress fields. In fact, when $r \to 0$, we have $K_0(r/\sqrt{c_k})|_{r\to 0} \to -\gamma + \ln(2\sqrt{c_k}/r)$, $K_1(r/\sqrt{c_k}) \to \sqrt{c_k}/r$, $K_2(r/\sqrt{c_k}) \to 2c_k/r^2 - 1/2$, $(k = 1, 2)$ and, thus, u_y is finite, $\varepsilon_{ij} \to 0$, $\sigma_{ij} \to 0$. The fields of displacements (10) and strains (11) have been discussed in detail in [8, 9] within a special version of gradient elasticity theory ($c_1 \equiv 0$). The stress fields (12) have been examined in [10]. It has been shown there that they attain their extreme values ($|\sigma_{xx}| \approx 0.45\,\mu$, $|\sigma_{yy}| \approx |\sigma_{xy}| \approx 0.27\,\mu$ and $|\sigma_{iz}| \approx 0.25\,\mu$ for $b_i = a = 4\sqrt{c_1}$ and $\nu = 0.3$) at a distance $\approx a/4$ from the dislocation line. Far away from the dislocation core ($r \geq r_0 \approx 4\sqrt{c_k}$), the gradient solutions coincide with the classical ones [8–10].

Using (12), one can find the elastic energy of the dislocation within the gradient elasticity given by (2) as follows [10]

$$
W = \frac{\mu}{4\pi(1-\nu)}\left\{\frac{b_x^2}{2} + [b_x^2 + (1-\nu)b_z^2]\left(\gamma + \ln\frac{R}{2\sqrt{c_1}}\right)\right\}, \qquad (13)
$$

where $\gamma = 0.57721566\ldots$ is Euler's constant. Thus, we obtain a strain energy expression which is not singular at the dislocation line.

3. Disclinations

3.1. CLASSICAL SOLUTION

Consider a disclination of general type with Frank vector $\boldsymbol{\omega} = \omega_x \boldsymbol{e}_x + \omega_y \boldsymbol{e}_y + \omega_z \boldsymbol{e}_z$ in an infinite elastic medium. The scalars ω_x and ω_y determine the twist components of the disclination while ω_z determines its wedge component. Let its line coincides with the z-axis of the above coordinate system. For such an isolated disclination, both classical and gradient solutions themselves have no physical meaning because they are not screened but they may be used in modeling screened disclination configurations as basic elements. The classical solution for elastic strain fields ε^0_{ij} reads [23] (in units of $1/[4\pi(1-\nu)]$)

$$\begin{aligned}
\varepsilon^0_{xx} &= \omega_x zx\frac{2\nu r^2 - x^2 + y^2}{r^4} + \omega_y zy\frac{2\nu r^2 - 3x^2 - y^2}{r^4} + \omega_z\left\{(1-2\nu)\ln r + \frac{y^2}{r^2}\right\},\\
\varepsilon^0_{yy} &= \omega_x zx\frac{2\nu r^2 - x^2 - 3y^2}{r^4} + \omega_y zy\frac{2\nu r^2 + x^2 - y^2}{r^4} + \omega_z\left\{(1-2\nu)\ln r + \frac{x^2}{r^2}\right\},\\
\varepsilon^0_{xy} &= (\omega_y x - \omega_x y)z\frac{x^2 - y^2}{r^4} - \omega_z\frac{xy}{r^2}, \quad \varepsilon^0_{xz} = \omega_y\frac{xy}{r^2} - \omega_x\left\{(1-2\nu)\ln r + \frac{y^2}{r^2}\right\},\\
\varepsilon^0_{yz} &= \omega_x\frac{xy}{r^2} - \omega_y\left\{(1-2\nu)\ln r + \frac{x^2}{r^2}\right\}, \qquad (14)
\end{aligned}$$

and for the stress fields it may be written (in units of $\mu/[2\pi(1-\nu)]$) as

$$\begin{aligned}
&\sigma^0_{xx} = \varepsilon^0_{xx}(\nu=0), \quad \sigma^0_{yy} = \varepsilon^0_{yy}(\nu=0), \quad \sigma^0_{xy} = \varepsilon^0_{xy}, \quad \sigma^0_{xz} = \varepsilon^0_{xz}, \quad \sigma^0_{yz} = \varepsilon^0_{yz},\\
&\sigma^0_{zz} = -\omega_x\, z\, 2\nu\frac{x}{r^2} - \omega_y\, z\, 2\nu\frac{y}{r^2} + \omega_z\, 2\nu\ln r\,. \qquad (15)
\end{aligned}$$

Most of the components in (14) and (15) contain singular terms $\sim \ln r$.

3.2. GRADIENT SOLUTION

The gradient solutions have been originally obtained for a disclination dipole within both the gradient theories considered in *Section 1.* Solving (4), we solve finally for an individual disclination under consideration the strain field [6] $\varepsilon_{ij} = \varepsilon^0_{ij} + \varepsilon^{gr}_{ij}$, where ε^0_{ij} are given by (14) and ε^{gr}_{ij} (in units of $1/[4\pi(1-\nu)]$) by

$$\begin{aligned}
\varepsilon^{gr}_{xx} &= \omega_x\, 2xz\left\{(y^2 - \nu r^2)\Phi_1 + (x^2 - 3y^2)\Phi_2\right\}\\
&+ \omega_y\, 2yz\left\{(y^2 - \nu r^2)\Phi_1 + (3x^2 - y^2)\Phi_2\right\} + \omega_z\left\{\Phi_0 + r^2(x^2 - y^2)\Phi_2\right\},\\
\varepsilon^{gr}_{yy} &= \omega_x\, 2xz\left\{(x^2 - \nu r^2)\Phi_1 - (x^2 - 3y^2)\Phi_2\right\}\\
&+ \omega_y\, 2yz\left\{(x^2 - \nu r^2)\Phi_1 - (3x^2 - y^2)\Phi_2\right\} + \omega_z\left\{\Phi_0 - r^2(x^2 - y^2)\Phi_2\right\},\\
\varepsilon^{gr}_{xy} &= \omega_x\, 2yz\left\{-x^2\Phi_1 + (3x^2 - y^2)\Phi_2\right\}\\
&- \omega_y\, 2xz\left\{y^2\Phi_1 + (x^2 - 3y^2)\Phi_2\right\} + \omega_z\, 2xyr^2\Phi_2,\\
\varepsilon^{gr}_{xz} &= \omega_x\left\{-\Phi_0 - r^2(x^2 - y^2)\Phi_2\right\} - \omega_y\, 2xyr^2\Phi_2,\\
\varepsilon^{gr}_{yz} &= \omega_y\left\{-\Phi_0 + r^2(x^2 - y^2)\Phi_2\right\} - \omega_x\, 2xyr^2\Phi_2, \qquad (16)
\end{aligned}$$

where Φ_i are the same as in *Section 2.2.* For the stress field, the solution of (5) gives [7] $\sigma_{ij} = \sigma^0_{ij} + \sigma^{gr}_{ij}$, where σ^0_{ij} are given by (15) and σ^{gr}_{ij} (in units of $\mu/[2\pi(1-\nu)]$) by

$$\begin{aligned}
&\sigma^{gr}_{xx} = \varepsilon^{gr}_{xx}(\nu=0, c_2 \leftrightarrow c_1), \quad \sigma^{gr}_{yy} = \varepsilon^{gr}_{yy}(\nu=0, c_2 \leftrightarrow c_1),\\
&\sigma^{gr}_{zz} = 2\nu\left\{(\omega_x x + \omega_y y)\, zr^2\Phi_1(c_2 \leftrightarrow c_1) + \omega_z\Phi_0(\nu=0, c_2 \leftrightarrow c_1)\right\},\\
&\sigma^{gr}_{xy} = \varepsilon^{gr}_{xy}(c_2 \leftrightarrow c_1), \quad \sigma^{gr}_{xz} = \varepsilon^{gr}_{xz}(c_2 \leftrightarrow c_1), \quad \sigma^{gr}_{yz} = \varepsilon^{gr}_{yz}(c_2 \leftrightarrow c_1). \qquad (17)
\end{aligned}$$

Using the limiting transitions noted in *Section 2.2*, it is easy to show the total elimination of classical logarithmic singularity from elastic fields (16) and (17). In [6, 7], we have considered similar elastic fields of disclination dipoles in detail and found that they are equal to zero or attain finite values at the disclination lines. The non-vanishing values depend strongly on the dipole arm, d, and exhibit a regular and monotonous (wedge disclinations) or non-monotonous (twist disclinations) behavior for short-range nanoscale ($d < 10\sqrt{c}$) interactions between disclinations. When the disclinations annihilate ($d \to 0$), the elastic strains and stresses tend to zero. Far from the disclination line ($r \gg 10\sqrt{c}$) gradient and classical solutions coincide. When $d \ll \sqrt{c}$, the elastic fields of a dipole of wedge disclinations transform into the elastic fields of an edge dislocation [9, 10] as is the case in the classical theory of elasticity.

4. Conclusions

The gradient elasticity described by (2) has been employed in the consideration of nanoscale short-range elastic fields and interactions of dislocations and disclinations. Exact analytical solutions for the displacements, strain and stress fields and elastic energies of dislocations have been reported which demonstrate the elimination of any singularity from the elastic fields and energies at the dislocation line. For disclinations, the gradient solutions have been given for the strain and stress fields where the classical singularities at the disclination lines also disappear. These new non-singular elastic fields are considered as especially useful for modeling nanoscale behavior and interactions of dislocations and disclinations in thin-film or nanostructured solids.

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